Author index to volume 203

Reineker, Superradiance of 2D Frenkel exciton-polaritons: mixing of molecular configu-	
rations and resonance interaction with the substrate	203 (1996) 11
Ågren, H., see Norman, P.	203 (1996) 23
Azriel, V.M., G.D. Billing, L.Yu. Rusin and M.B. Sevryuk, A test of the semiclassical Wigner method for the reaction $F + H_2 \rightarrow H + HF$ (Chemical Physics 195 (1995)	
243–258)	203 (1996) 279
Bähr, A., G. Cooper, J.C. Green, K.A. Longley, M. Lovell-Smith and G.S. McGrady, Origins of structure in the e ₁ ionisation bands of magnesocene and osmocene. A	
photoelectron spectroscopic study of $M(\eta - C_5D_5)_2$, $M = Mg$ and Os	203 (1996) 223
Baines, K.M., see Xiong, J.Z.	203 (1996) 81
Bancewicz, M., Density of levels in vibrational spectra of molecules. Coupled Morse	
oscillators	203 (1996) 93
Bartels, D.M. and E. Roduner, Reaction of H, D, and muonium atoms with I in aqueous	
solution	203 (1996) 339
Bennema, P., see Vogels, L.J.P.	203 (1996) 69
Berriche, H. and F.X. Gadea, Ab initio study of the LiH ⁺ molecule, electronic interaction	
analysis and LiH UV photoelectron spectrum (Chemical Physics 191 (1995) 119-131)	203 (1996) 373
Besnard, M., see Zoidis, E.	203 (1996) 233
Billing, G.D., see Azriel, V.M.	203 (1996) 279
Blanks, R.F., see Vogels, L.J.P.	203 (1996) 69
Bolton, K. and S. Nordholm, A classical molecular dynamics study of the intramolecular	
energy transfer of model trans-stilbene	203 (1996) 101
Brion, C.E., see Ibuki, T.	203 (1996) 359
Bulanin, K.M., M.O. Bulanin and A.A. Tsyganenko, Infrared spectra of ¹⁸ O-enriched	
ozones in liquid oxygen solution	203 (1996) 127
Bulanin, M.O., see Bulanin, K.M.	203 (1996) 127
Buss, V. and K. Kolster, Electronic structure calculations on helicenes. Concerning the	
chirality of helically twisted aromatic systems	203 (1996) 309
Cooper, G., see Bähr, A.	203 (1996) 223
Coutinho-Neto, M.D. and A.A.S. da Gama, Donor-acceptor interaction in two-level-re-	
duced molecular systems	203 (1996) 43
Da Gama, A.A.S., see Coutinho-Neto, M.D.	203 (1996) 43
Doktorov, A.B., see Spirina, O.B.	203 (1996) 177
Dubovsky, O.A., see Agranovich, V.M.	203 (1996) 11
, , , , , , , , , , , , , , , , , , , ,	

Fahr, A. and A. Nayak, Temperature dependent ultraviolet absorption cross sections of	
propylene, methylacetylene and vinylacetylene	203 (1996) 351
Gadea, F.X., see Berriche, H.	203 (1996) 373
Green, J.C., see Bähr, A.	203 (1996) 223
Green, J.C., see Ketkov, S.Yu.	203 (1996) 245
Grigorishin, K.I., see Agranovich, V.M.	203 (1996) 11
Grimbergen, R.F.P., see Vogels, L.J.P.	203 (1996) 69
Hada, M., see Higashioji, T.	203 (1996) 159
Higashioji, T., M. Hada, M. Sugimoto and H. Nakatsuji, Basis set dependence of magnetic	
shielding constant calculated by the Hartree-Fock/finite perturbation method	203 (1996) 159
Hikida, T., see Hikosaka, Y.	203 (1996) 137
Hikosaka, Y. and T. Hikida, Electronic energy relaxation of benzophenone vapor	203 (1996) 137
Hirata, F., see Kawata, M.	203 (1996) 53
Hiraya, A., see Ibuki, T.	203 (1996) 359
Hitchcock, A.P., see Xiong, J.Z.	203 (1996) 81
Ibuki, T., A. Hiraya, T.N. Olney and C.E. Brion, Ionic photofragmentation (11.5–160 eV) and PIPICO spectroscopy (40–130 eV) of BrCN in the valence shell and bromine 3d	
regions	203 (1996) 359
Jiang, D.T., see Xiong, J.Z.	203 (1996) 81
Jonsson, D., see Norman, P.	203 (1996) 23
Joyeux, M., Classical dynamics of the 1:1, 1:2 and 1:3 resonance Hamiltonians	203 (1996) 281
Kato, S., see Kawata, M.	203 (1996) 53
Kauffmann, H.F., see Pálszegi, T.	203 (1996) 143
Kawata, M., S. Ten-no, S. Kato and F. Hirata, Theoretical study for the basicities of methylamines in aqueous solution: A RISM-SCF calculation of solvation thermodynam-	202 (1005) 72
ics	203 (1996) 53
Ketkov, S.Yu., C. Mehnert and J.C. Green, Electronic excited states of bis(η^6 -arene)tungsten: an investigation by ultraviolet photoabsorption spectroscopy in the vapour and	
solution phases	203 (1996) 245
Kolster, K., see Buss, V.	203 (1996) 309
Leskova, T.A., see Agranovich, V.M.	203 (1996) 11
Liu, Z.F., see Xiong, J.Z.	203 (1996) 81
Longley, K.A., see Bähr, A.	203 (1996) 223
Lovell-Smith, M., see Bähr, A.	203 (1996) 223
McGrady, G.S., see Bähr, A.	203 (1996) 223
Meath, W.J., see Wheatley, R.J.	203 (1996) 209
Mehnert, C., see Ketkov, S.Yu.	203 (1996) 245
Meluš, M., see Pálszegi, T.	203 (1996) 143
Nakashima, K., see Tokeshi, M.	203 (1996) 257
Nakatsuji, H., see Higashioji, T.	203 (1996) 159

Neural A con Take A	202 (1004) 251
Nayak, A., see Fahr, A. Neidlinger, Th., see Agranovich, V.M.	203 (1996) 351
Nordholm, S., see Bolton, K.	203 (1996) 11
Norman, P., D. Jonsson, O. Vahtras and H. Ågren, Non-linear electric and magnetic	203 (1996) 101
properties obtained from cubic response functions in the random phase approximation	203 (1996) 23
Ogawa, T., see Tokeshi, M.	203 (1996) 257
Ohno, M., Anomalous Auger decay in adsorbates	203 (1996) 1
Olney, T.N., see Ibuki, T.	203 (1996) 359
Pálszegi, T., J. Rychlý, M. Meluš and H.F. Kauffmann, Excitation migration and transfer to interstitial traps – low dimensional transport and conformational motion	203 (1996) 143
Delaster D. and Americal VIII	202 (1006) 11
Reineker, P., see Agranovich, V.M.	203 (1996) 11
Roberts, S.A., see Vogels, L.J.P.	203 (1996) 69
Roduner, E., see Bartels, D.M.	203 (1996) 339
Roduner, E., see Tregenna-Piggott, P.L.W. Rusin, L.Yu., see Azriel, V.M.	203 (1996) 317
Rychlý, J., see Pálszegi, T.	203 (1996) 279
Rychly, J., see Paiszegi, 1.	203 (1996) 143
Santos, S., see Tregenna-Piggott, P.L.W.	203 (1996) 317
Sevryuk, M.B., see Azriel, V.M.	203 (1996) 279
Sham, T.K., see Xiong, J.Z.	203 (1996) 81
Spirina, O.B. and A.B. Doktorov, The steady-state Green's function method in unimolec-	
ular reactions. Generalization of the MFPT concept. I. Irreversible reactions	203 (1996) 177
Strom, C.S., see Vogels, L.J.P.	203 (1996) 69
Sugawara, Ki., see Trushin, S.A.	203 (1996) 267
Sugimoto, M., see Higashioji, T.	203 (1996) 159
Takeo, H., see Trushin, S.A.	203 (1996) 267
Ten-no, S., see Kawata, M.	203 (1996) 53
Tokeshi, M., K. Nakashima and T. Ogawa, Dissociation of aliphatic hydrocarbons by controlled electron impact: Vibrational and rotational energy distributions of the excited	
CH radicals	203 (1996) 257
Tregenna-Piggott, P.L.W., E. Roduner and S. Santos, Calculation of the avoided level- crossing muon spin resonance response for various stochastic motions using Monte	
Carlo methods	203 (1996) 317
Trushin, S.A., Ki. Sugawara and H. Takeo, Formation of Cr atoms in the 5 µm	
multiphoton decomposition of Cr(CO) ₆	203 (1996) 267
Tsyganenko, A.A., see Bulanin, K.M.	203 (1996) 127
Tyliszczak, T., see Xiong, J.Z.	203 (1996) 81
Urquhart, S.G., see Xiong, J.Z.	203 (1996) 81
Vahtras, O., see Norman, P.	203 (1996) 23
Vogels, L.J.P., R.F.P. Grimbergen, C.S. Strom, P. Bennema, S.A. Roberts and R.F. Blanks,	
On the theoretical and experimental morphology of paraxylene	203 (1996) 69

Wen, A.T., see Xiong, J.Z.
Wheatley, R.J. and W.J. Meath, Dispersion and induction energy damping functions, and their scale with interspecies distance, for the interaction of H⁻ with H, He and Li atoms
Xiong, J.Z., D.T. Jiang, Z.F. Liu, K.M. Baines, T.K. Sham, S.G. Urquhart, A.T. Wen, T. Tyliszczak and A.P. Hitchcock, Si core-level excitation of hexamethyldisilane studied by synchrotron radiation and multiple-scattering X α calculation
Yarwood, J., see Zoidis, E.
Zoidis, E., M. Besnard and J. Yarwood, Far infrared spectroscopic studies of the molecular dynamics and interactions of pyridine in organic solvents
203 (1996) 81
203 (1996) 233

Subject index to volume 203

Physics 195 (1995) 243–258), V.M. Azriel, G.D. Billing, L.Yu. Rusin and M.B.	
Sevryuk	203 (1996) 279
Classical dynamics of the 1:1, 1:2 and 1:3 resonance Hamiltonians, M. Joyeux	203 (1996) 281
Electronic structure calculations on helicenes. Concerning the chirality of helically twisted	
aromatic systems, V. Buss and K. Kolster	203 (1996) 309
Calculation of the avoided level-crossing muon spin resonance response for various stochastic motions using Monte Carlo methods, P.L.W. Tregenna-Piggott, E. Roduner and S. Santos	203 (1996) 317
Reaction of H, D, and muonium atoms with I ⁻ in aqueous solution, D.M. Bartels and E.	203 (1990) 317
Reaction of 11, 15, and indomain atoms with 1 in aqueous solution, 15.1vi. Barters and E.	203 (1996) 339
Temperature dependent ultraviolet absorption cross sections of propylene, methylacetylene	203 (1990) 339
and vinylacetylene, A. Fahr and A. Nayak	203 (1996) 351
Ab initio study of the LiH ⁺ molecule, electronic interaction analysis and LiH UV	203 (1990) 331
photoelectron spectrum (Chemical Physics 191 (1995) 119–131), H. Berriche and F.X.	
Gadea	203 (1996) 373
Ionic photofragmentation (11.5–160 eV) and PIPICO spectroscopy (40–130 eV) of BrCN	203 (1770) 373
in the valence shell and bromine 3d regions, T. Ibuki, A. Hiraya, T.N. Olney and C.E.	
Brion	203 (1996) 359
Methods	
Theoretical	
Many body and quasiparticle approaches	
Anomalous Auger decay in adsorbates, M. Ohno	203 (1996) 1
Superradiance of 2D Frenkel exciton-polaritons: mixing of molecular configurations and	
resonance interaction with the substrate, V.M. Agranovich, O.A. Dubovsky, K.I. Grigo-	
rishin, T.A. Leskova, Th. Neidlinger and P. Reineker	203 (1996) 11
Excitation migration and transfer to interstitial traps - low dimensional transport and	
conformational motion, T. Pálszegi, J. Rychlý, M. Meluš and H.F. Kauffmann	203 (1996) 143
Coupling schemes and perturbative treatments	
Non-linear electric and magnetic properties obtained from cubic response functions in the	()
random phase approximation, P. Norman, D. Jonsson, O. Vahtras and H. Agren	203 (1996) 23
Donor-acceptor interaction in two-level-reduced molecular systems, M.D. Coutinho-Neto	**** (*****)
and A.A.S. da Gama	203 (1996) 43

Basis set dependence of magnetic shielding constant calculated by the Hartree-Fock/finite perturbation method, T. Higashioji, M. Hada, M. Sugimoto and H. Nakatsuji	203 (1996) 159
Equilibrium statistical mechanics	
Theoretical study for the basicities of methylamines in aqueous solution: A RISM-SCF calculation of solvation thermodynamics, M. Kawata, S. Ten-no, S. Kato and F. Hirata On the theoretical and experimental morphology of paraxylene, L.J.P. Vogels, R.F.P.	203 (1996) 53
Grimbergen, C.S. Strom, P. Bennema, S.A. Roberts and R.F. Blanks	203 (1996) 69
Statistical mechanics of stationary states	
Excitation migration and transfer to interstitial traps – low dimensional transport and conformational motion, T. Pálszegi, J. Rychlý, M. Meluš and H.F. Kauffmann The steady-state Green's function method in unimolecular reactions. Generalization of the	203 (1996) 143
MFPT concept. I. Irreversible reactions, O.B. Spirina and A.B. Doktorov	203 (1996) 177
Ab initio schemes for stationary properties	
Non-linear electric and magnetic properties obtained from cubic response functions in the random phase approximation, P. Norman, D. Jonsson, O. Vahtras and H. Ågren Theoretical study for the basicities of methylamines in aqueous solution: A RISM-SCF	203 (1996) 23
calculation of solvation thermodynamics, M. Kawata, S. Ten-no, S. Kato and F. Hirata	203 (1996) 53
Basis set dependence of magnetic shielding constant calculated by the Hartree-Fock/finite perturbation method, T. Higashioji, M. Hada, M. Sugimoto and H. Nakatsuji Dispersion and induction energy damping functions, and their scale with interspecies	203 (1996) 159
distance, for the interaction of H ⁻ with H, He and Li atoms, R.J. Wheatley and W.J. Meath	203 (1996) 209
Computational and simulation methods	
Si core-level excitation of hexamethyldisilane studied by synchrotron radiation and multi-	
ple-scattering $X\alpha$ calculation, J.Z. Xiong, D.T. Jiang, Z.F. Liu, K.M. Baines, T.K.	
Sham, S.G. Urquhart, A.T. Wen, T. Tyliszczak and A.P. Hitchcock	203 (1996) 81
Density of levels in vibrational spectra of molecules. Coupled Morse oscillators, M. Bancewicz	203 (1996) 93
Dispersion and induction energy damping functions, and their scale with interspecies distance, for the interaction of H ⁻ with H, He and Li atoms, R.J. Wheatley and W.J.	200 (1770) 70
Meath	203 (1996) 209
Melandar dynamics and scattering theory	
Molecular dynamics and scattering theory A classical molecular dynamics study of the intramolecular energy transfer of model	
trans-stilbene, K. Bolton and S. Nordholm	203 (1996) 101
Experimental	
Infrared spectroscopy	
Infrared spectra of ¹⁸ O-enriched ozones in liquid oxygen solution, K.M. Bulanin, M.O.	
Bulanin and A.A. Tsyganenko	203 (1996) 127
Far infrared spectroscopic studies of the molecular dynamics and interactions of pyridine in organic solvents, E. Zoidis, M. Besnard and J. Yarwood	203 (1996) 233

Visible and UV spectroscopy

- Electronic excited states of bis(η^6 -arene)tungsten: an investigation by ultraviolet photoabsorption spectroscopy in the vapour and solution phases, S.Yu. Ketkov, C. Mehnert and J.C. Green
- 203 (1996) 245

Photoelectron and Auger spectroscopy

- Anomalous Auger decay in adsorbates, M. Ohno
- Origins of structure in the e_1 ionisation bands of magnesocene and osmocene. A photoelectron spectroscopic study of $M(\eta-C_5D_5)_2$, M=Mg and Os, A. Bähr, G. Cooper, J.C. Green, K.A. Longley, M. Lovell-Smith and G.S. McGrady
- 203 (1996) 1 203 (1996) 223

Electron impact spectroscopy

Dissociation of aliphatic hydrocarbons by controlled electron impact: Vibrational and rotational energy distributions of the excited CH radicals, M. Tokeshi, K. Nakashima and T. Ogawa

203 (1996) 257

Laser methods

Formation of Cr atoms in the 5 µm multiphoton decomposition of Cr(CO)₆, S.A. Trushin, K.-i. Sugawara and H. Takeo

203 (1996) 267

Synchrotron spectroscopies

Si core-level excitation of hexamethyldisilane studied by synchrotron radiation and multiple-scattering $X\alpha$ calculation, J.Z. Xiong, D.T. Jiang, Z.F. Liu, K.M. Baines, T.K. Sham, S.G. Urquhart, A.T. Wen, T. Tyliszczak and A.P. Hitchcock

203 (1996) 81

Atomic and molecular beam techniques

Dissociation of aliphatic hydrocarbons by controlled electron impact: Vibrational and rotational energy distributions of the excited CH radicals, M. Tokeshi, K. Nakashima and T. Ogawa

203 (1996) 257

Time-resolved experiments

- Electronic energy relaxation of benzophenone vapor, Y. Hikosaka and T. Hikida
- Formation of Cr atoms in the 5 µm multiphoton decomposition of Cr(CO)₆, S.A. Trushin, K.-i. Sugawara and H. Takeo

203 (1996) 137

203 (1996) 267

Measurement of macroscopic variables

On the theoretical and experimental morphology of paraxylene, L.J.P. Vogels, R.F.P. Grimbergen, C.S. Strom, P. Bennema, S.A. Roberts and R.F. Blanks

203 (1996) 69

Objects

Bulk systems

Liquids neat

- The steady-state Green's function method in unimolecular reactions. Generalization of the MFPT concept. I. Irreversible reactions, O.B. Spirina and A.B. Doktorov
- 203 (1996) 177

Liquid mixtures and solutions	
Theoretical study for the basicities of methylamines in aqueous solution: A RISM-SCF calculation of solvation thermodynamics, M. Kawata, S. Ten-no, S. Kato and F. Hirata Infrared spectra of ¹⁸ O-enriched ozones in liquid oxygen solution, K.M. Bulanin, M.O.	203 (1996) 53
Bulanin and A.A. Tsyganenko	203 (1996) 127
Far infrared spectroscopic studies of the molecular dynamics and interactions of pyridine in organic solvents, E. Zoidis, M. Besnard and J. Yarwood	203 (1996) 233
Crystals	
On the theoretical and experimental morphology of paraxylene, L.J.P. Vogels, R.F.P. Grimbergen, C.S. Strom, P. Bennema, S.A. Roberts and R.F. Blanks	203 (1996) 69
Polymers	
Non-linear electric and magnetic properties obtained from cubic response functions in the random phase approximation, P. Norman, D. Jonsson, O. Vahtras and H. Ågren	203 (1996) 23
Low-dimensional materials	
Superradiance of 2D Frenkel exciton-polaritons: mixing of molecular configurations and resonance interaction with the substrate, V.M. Agranovich, O.A. Dubovsky, K.I. Grigorishin, T.A. Leskova, Th. Neidlinger and P. Reineker	203 (1996) 11
Microscopic systems	
Molecules (neutral and ionic)	
Anomalous Auger decay in adsorbates, M. Ohno	203 (1996) 1
Density of levels in vibrational spectra of molecules. Coupled Morse oscillators, M. Bancewicz	203 (1996) 93
Dispersion and induction energy damping functions, and their scale with interspecies	203 (1990) 93
distance, for the interaction of H ⁻ with H, He and Li atoms, R.J. Wheatley and W.J.	
Meath	203 (1996) 209
Electronic excited states of bis(η^6 -arene)tungsten: an investigation by ultraviolet photoabsorption spectroscopy in the vapour and solution phases, S.Yu. Ketkov, C. Mehnert and	
J.C. Green	203 (1996) 245
Formation of Cr atoms in the 5 μm multiphoton decomposition of Cr(CO) ₆ , S.A. Trushin, Ki. Sugawara and H. Takeo	203 (1996) 267
-small polyatomics	
Non-linear electric and magnetic properties obtained from cubic response functions in the random phase approximation, P. Norman, D. Jonsson, O. Vahtras and H. Ågren	203 (1996) 23
Si core-level excitation of hexamethyldisilane studied by synchrotron radiation and multiple-scattering $X\alpha$ calculation, J.Z. Xiong, D.T. Jiang, Z.F. Liu, K.M. Baines, T.K.	
Sham, S.G. Urquhart, A.T. Wen, T. Tyliszczak and A.P. Hitchcock A classical molecular dynamics study of the intramolecular energy transfer of model	203 (1996) 81
trans-stilbene, K. Bolton and S. Nordholm	203 (1996) 101
Infrared spectra of ¹⁸ O-enriched ozones in liquid oxygen solution, K.M. Bulanin, M.O. Bulanin and A.A. Tsyganenko	203 (1996) 127
Basis set dependence of magnetic shielding constant calculated by the Hartree-Fock/finite perturbation method, T. Higashioji, M. Hada, M. Sugimoto and H. Nakatsuji	203 (1996) 159

Far infrared spectroscopic studies of the molecular dynamics and interactions of pyridine in organic solvents, E. Zoidis, M. Besnard and J. Yarwood Dissociation of aliphatic hydrocarbons by controlled electron impact: Vibrational and	203 (1996) 233
rotational energy distributions of the excited CH radicals, M. Tokeshi, K. Nakashima and T. Ogawa	203 (1996) 257
-aromatics	
On the theoretical and experimental morphology of paraxylene, L.J.P. Vogels, R.F.P.	202 (1004) 40
Grimbergen, C.S. Strom, P. Bennema, S.A. Roberts and R.F. Blanks Electronic energy relaxation of benzophenone vapor, Y. Hikosaka and T. Hikida	203 (1996) 69 203 (1996) 137
Electronic energy relaxation of benzophenone vapor, 1. Throsaka and 1. Thrida	203 (1990) 137
-other large	
Origins of structure in the e_1 ionisation bands of magnesocene and osmocene. A photo- electron spectroscopic study of $M(\eta-C_5D_5)_2$, $M=Mg$ and Os, A. Bähr, G. Cooper, J.C. Green, K.A. Longley, M. Lovell-Smith and G.S. McGrady	203 (1996) 223
Electronic excited states of bis(η^6 -arene)tungsten: an investigation by ultraviolet photoab-	
sorption spectroscopy in the vapour and solution phases, S.Yu. Ketkov, C. Mehnert and J.C. Green	203 (1996) 245
Molecular aggregates	
-dimers	
Donor-acceptor interaction in two-level-reduced molecular systems, M.D. Coutinho-Neto and A.A.S. da Gama	203 (1996) 43
-van der Waals molecules	
Dispersion and induction energy damping functions, and their scale with interspecies	
distance, for the interaction of H ⁻ with H, He and Li atoms, R.J. Wheatley and W.J. Meath	203 (1996) 209
Quasiparticles (including excitons)	
Superradiance of 2D Frenkel exciton-polaritons: mixing of molecular configurations and	
resonance interaction with the substrate, V.M. Agranovich, O.A. Dubovsky, K.I. Grigorishin, T.A. Leskova, Th. Neidlinger and P. Reineker	203 (1996) 11
Excitation migration and transfer to interstitial traps – low dimensional transport and	203 (1770) 11
conformational motion, T. Pálszegi, J. Rychlý, M. Meluš and H.F. Kauffmann	203 (1996) 143
Phenomena	
Molecular structure Density of levels in vibrational spectra of molecules. Coupled Morse oscillators, M.	
Bancewicz	203 (1996) 93
Vibrations and rotations of molecules	
Density of levels in vibrational spectra of molecules. Coupled Morse oscillators, M.	
Bancewicz	203 (1996) 93

Dissociation of aliphatic hydrocarbons by controlled electron impact: Vibrational and rotational energy distributions of the excited CH radicals, M. Tokeshi, K. Nakashima	()
and T. Ogawa	203 (1996) 257
Electronic structure and states	203 (1996) 1
Anomalous Auger decay in adsorbates, M. Ohno Superradiance of 2D Frenkel exciton-polaritons: mixing of molecular configurations and resonance interaction with the substrate, V.M. Agranovich, O.A. Dubovsky, K.I. Grigo-	203 (1990) 1
rishin, T.A. Leskova, Th. Neidlinger and P. Reineker	203 (1996) 11
Theoretical study for the basicities of methylamines in aqueous solution: A RISM-SCF calculation of solvation thermodynamics, M. Kawata, S. Ten-no, S. Kato and F. Hirata	203 (1996) 53
Si core-level excitation of hexamethyldisilane studied by synchrotron radiation and multiple-scattering $X\alpha$ calculation, J.Z. Xiong, D.T. Jiang, Z.F. Liu, K.M. Baines, T.K.	***********
Sham, S.G. Urquhart, A.T. Wen, T. Tyliszczak and A.P. Hitchcock Origins of structure in the e ₁ ionisation bands of magnesocene and osmocene. A photo-	203 (1996) 81
electron spectroscopic study of $M(\eta - C_5D_5)_2$, $M = Mg$ and Os, A. Bähr, G. Cooper, J.C. Green, K.A. Longley, M. Lovell-Smith and G.S. McGrady	203 (1996) 223
Electronic excited states of bis(η^6 -arene)tungsten: an investigation by ultraviolet photoab-	
sorption spectroscopy in the vapour and solution phases, S.Yu. Ketkov, C. Mehnert and J.C. Green	203 (1996) 245
Electric and magnetic properties	
Basis set dependence of magnetic shielding constant calculated by the Hartree-Fock/finite perturbation method, T. Higashioji, M. Hada, M. Sugimoto and H. Nakatsuji	203 (1996) 159
Molecular interactions	
Dispersion and induction energy damping functions, and their scale with interspecies	
distance, for the interaction of H ⁻ with H, He and Li atoms, R.J. Wheatley and W.J. Meath	203 (1996) 209
Spectral bandshapes and intensities	
Infrared spectra of ¹⁸ O-enriched ozones in liquid oxygen solution, K.M. Bulanin, M.O.	
Bulanin and A.A. Tsyganenko	203 (1996) 127
Far infrared spectroscopic studies of the molecular dynamics and interactions of pyridine in organic solvents, E. Zoidis, M. Besnard and J. Yarwood	203 (1996) 233
Energy transfer processes	
Electronic energy relaxation of benzophenone vapor, Y. Hikosaka and T. Hikida	203 (1996) 137
Excitation migration and transfer to interstitial traps – low dimensional transport and conformational motion, T. Pálszegi, J. Rychlý, M. Meluš and H.F. Kauffmann	203 (1996) 143
Molecular photophysical processes	
A classical molecular dynamics study of the intramolecular energy transfer of model	
trans-stilbene, K. Bolton and S. Nordholm	203 (1996) 101
Formation of Cr atoms in the 5 μm multiphoton decomposition of Cr(CO) ₆ , S.A. Trushin, Ki. Sugawara and H. Takeo	203 (1996) 267

Intramolecular dynamics

-vibrational energy redistribution (including vibrational dissociation) A classical molecular dynamics study of the intramolecular energy transfer of model trans-stilbene, K. Bolton and S. Nordholm	203 (1996) 101
Luminescence spectra, yields and lifetimes	
Superradiance of 2D Frenkel exciton-polaritons: mixing of molecular configurations and resonance interaction with the substrate, V.M. Agranovich, O.A. Dubovsky, K.I. Grigo-	
rishin, T.A. Leskova, Th. Neidlinger and P. Reineker	203 (1996) 11
Electronic energy relaxation of benzophenone vapor, Y. Hikosaka and T. Hikida	203 (1996) 137
Non-linear responses (including optical)	
Non-linear electric and magnetic properties obtained from cubic response functions in the random phase approximation, P. Norman, D. Jonsson, O. Vahtras and H. Ågren	203 (1996) 23
Reactions (including dissociation)	
-gas phase	
Dissociation of aliphatic hydrocarbons by controlled electron impact: Vibrational and rotational energy distributions of the excited CH radicals, M. Tokeshi, K. Nakashima	
and T. Ogawa	203 (1996) 257
Formation of Cr atoms in the 5 μm multiphoton decomposition of Cr(CO) ₆ , S.A. Trushin, Ki. Sugawara and H. Takeo	203 (1996) 267
-condensed phase	
The steady-state Green's function method in unimolecular reactions. Generalization of the MFPT concept. I. Irreversible reactions, O.B. Spirina and A.B. Doktorov	203 (1996) 177
-photochemical	
The steady-state Green's function method in unimolecular reactions. Generalization of the MFPT concept. I. Irreversible reactions, O.B. Spirina and A.B. Doktorov	203 (1996) 177
Electron transfer	
Donor-acceptor interaction in two-level-reduced molecular systems, M.D. Coutinho-Neto	
and A.A.S. da Gama	203 (1996) 43
Ionization (including Rydberg states)	
Anomalous Auger decay in adsorbates, M. Ohno	203 (1996) 1
Origins of structure in the e_1 ionisation bands of magnesocene and osmocene. A photo-electron spectroscopic study of $M(\eta - C_5D_5)_2$, $M = Mg$ and Os, A. Bähr, G. Cooper, J.C.	
Green, K.A. Longley, M. Lovell-Smith and G.S. McGrady	203 (1996) 223
Molecular motion (including diffusive)	
Excitation migration and transfer to interstitial traps – low dimensional transport and	203 (1996) 143
conformational motion, T. Pálszegi, J. Rychlý, M. Meluš and H.F. Kauffmann The steady-state Green's function method in unimolecular reactions. Generalization of the	203 (1990) 143
MFPT concept. I. Irreversible reactions, O.B. Spirina and A.B. Doktorov	203 (1996) 177

Far infrared spectroscopic studies of the molecular dynamics and interactions of pyridine in organic solvents, E. Zoidis, M. Besnard and J. Yarwood 203 (1996) 233 Isotopic effects Infrared spectra of ¹⁸O-enriched ozones in liquid oxygen solution, K.M. Bulanin, M.O. Bulanin and A.A. Tsyganenko 203 (1996) 127 Origins of structure in the e₁ ionisation bands of magnesocene and osmocene. A photoelectron spectroscopic study of $M(\eta - C_5D_5)_2$, M = Mg and Os, A. Bähr, G. Cooper, J.C. Green, K.A. Longley, M. Lovell-Smith and G.S. McGrady 203 (1996) 223 Thermodynamic and transport properties Theoretical study for the basicities of methylamines in aqueous solution: A RISM-SCF calculation of solvation thermodynamics, M. Kawata, S. Ten-no, S. Kato and F. Hirata 203 (1996) 53 Structure of solids and liquids On the theoretical and experimental morphology of paraxylene, L.J.P. Vogels, R.F.P.

203 (1996) 69

Grimbergen, C.S. Strom, P. Bennema, S.A. Roberts and R.F. Blanks

